

# Quantum Phase Transition in a Graphene Model

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**Abstract.** We present results for the equation of state of a graphene-like model in an effort to understand the properties of its quantum phase transition. The  $N_f$  fermion species interact through a three dimensional instantaneous Coulomb potential. Since there are no reliable analytical tools that work for all values of  $N_f$  and the coupling constant  $g$ , we rely on Monte Carlo simulations to calculate the critical properties of the model near the phase transition. We consider the four-component formulation for the fermion elds, which arises naturally as the continuum limit of the staggered fermion construction in (2+1) dimensions. In the limit of infinitely strong Coulomb interaction, the system undergoes a quantum phase transition at a critical number of fermion species  $N_{fc} \approx 4.7$ . We also calculate the values of the critical exponents at the quantum phase transition.

## 1. Introduction

There has been considerable recent interest in graphene sparked by its discovery and subsequent experimental study. In brief, for a carbon monolayer having one mobile electron per atom, a simple tight-binding model shows that the spectrum of low-energy excitations exhibits a linear dispersion relation centred on zeroes located at the six corners of the first Brillouin zone (see e.g. [1]). Using a linear transformation among the fields at two independent zeroes it is possible to recast the Hamiltonian in Dirac form with  $N_f = 2$  flavors of four-component spinor  $\psi$ , the counting of the massless degrees of freedom coming from 2 carbon atoms per unit cell  $\times$  2 zeroes per zone  $\times$  2 physical spin components per electron. Electron propagation in the graphene layer is thus relativistic, albeit at a speed  $v_F \approx c/100$ . Although this is a factor of 100 slower than the speed of light in vacuum, it is still much faster than the speed of electrons in an ordinary conductor. The implications for the high mobility of the resulting charge carriers (which may be negatively-charged “particles” or positively-charged “holes” depending on doping) is the source of the current excitement. The stability of the zero-energy points is topological in origin, as emphasised by Creutz [2].

While the above considerations apply quite generally, a realistic model of graphene must incorporate interactions between charge carriers. One such model, due to Son [3], has  $N_f$  massless fermion flavors propagating in the plane, but interacting via an instantaneous 3d Coulomb interaction. In Euclidean metric and static gauge  $\partial_0 A_0 = 0$  the action reads

$$S_1 = \sum_{a=1}^{N_f} \int dx_0 d^2x (\bar{\psi}_a \gamma_0 \partial_0 \psi_a + v_F \bar{\psi}_a \vec{\gamma} \cdot \vec{\nabla} \psi_a + iV \bar{\psi}_a \gamma_0 \psi_a) + \frac{1}{2e^2} \int dx_0 d^3x (\partial_i V)^2, \quad (1)$$

where  $e$  is the electron charge,  $V \equiv A_0$ , and the  $4 \times 4$  Dirac matrices satisfy  $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$ ,  $\mu = 0, 1, 2, 3$ . In our notation  $\vec{x}$  is a vector in the  $2d$  plane while the index  $i$  runs over all three spatial directions. In the large- $N_f$  limit the dominant quantum correction  $\Pi(p)$  comes from a vacuum polarisation fermion- antifermion loop and the resummed  $V$  propagator becomes

$$D_1(p) = (D_0^{-1}(p) - \Pi(p))^{-1} = \left( \frac{2|\vec{p}|}{e^2} + \frac{N_f}{8} \frac{|\vec{p}|^2}{(p^2)^{\frac{1}{2}}} \right)^{-1}, \quad (2)$$

where  $p^2 = (p_0, \vec{p})^2 \equiv p_0^2 + v_F^2 |\vec{p}|^2$ , and  $D_0(p)$  corresponds to the classical propagation of  $V$ . In either the strong coupling or large- $N_f$  limits  $D_1(p)$  is thus dominated by  $\Pi(p)$ , the relative importance of the original Coulomb interaction being governed by a parameter  $\lambda \equiv |\Pi/D_0|_{p_0=0}$ .

The chiral symmetry breaking, due to the spontaneous condensation of particle - hole pairs, is signalled by an order parameter  $\langle \bar{\psi}\psi \rangle \neq 0$ . Physically the most important outcome is the generation of a gap in the fermion spectrum, implying the model is an insulator. Son [3] postulates that this insulating phase exists in the corner of the phase diagram corresponding to large  $e^2$  and small  $N_f$ , and in particular that the insulator-conductor phase transition taking place at  $N_f = N_{fc}$  in the strong-coupling limit  $e^2 \rightarrow \infty$  is a novel quantum critical point. The value of  $N_{fc}$ , and the issue of whether it is greater or less than the physical value  $N_f = 2$ , must be settled by a non-perturbative calculation. A recent estimate obtained by a renormalisation group treatment of radiatively-induced four-fermion contact interactions, is  $N_{fc} = 2.03$  [4].

The proposed physics is very reminiscent of the three dimensional Thirring model, which is analytically tractable at large  $N_f$ , but exhibits spontaneous chiral symmetry breaking at small  $N_f$  and strong coupling [5, 6]. Arguably the Thirring model is the simplest field theory of fermions requiring a computational solution: the location of the phase transition at  $N_f = N_{fc}$  in the strong coupling limit has recently been determined by lattice simulations to be  $N_{fc} = 6.6(1)$  [7]. The apparent similarity of the two systems has led us to propose a Thirring-like model pertinent to graphene, with Lagrangian

$$S_2 = \sum_{a=1}^{N_f} \int dx_0 d^2x \left[ \bar{\psi}_a \gamma_\mu \partial_\mu \psi_a + iV \bar{\psi}_a \gamma_0 \psi_a + \frac{1}{2g^2} V^2 \right]. \quad (3)$$

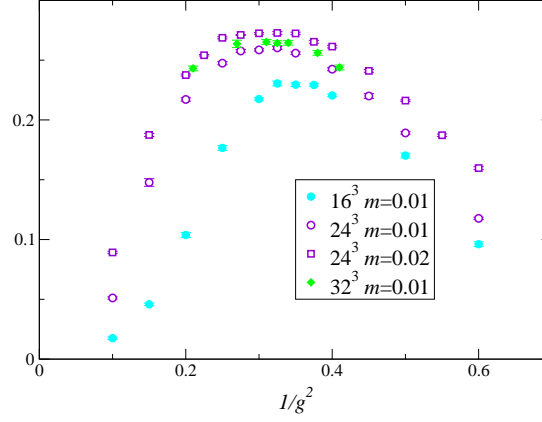
As for (1) we assume a large- $N_f$  limit to estimate the dominant vacuum polarisation correction; the resultant propagator for  $V$  is

$$D_2(p) = \left( \frac{1}{g^2} + \frac{N_f}{8} \frac{|\vec{p}|^2}{(p^2)^{\frac{1}{2}}} \right)^{-1}. \quad (4)$$

In the strong-coupling or large- $N_f$  limits,  $D_2$  coincides with  $D_1$ , implying that the fermion interactions are equivalent. It is also the case that  $\lim_{p \rightarrow \infty} D_2(p) = \lim_{\lambda \rightarrow \infty} D_1(p)$ . This last limit is important because critical behaviour in the Thirring model is governed by a UV-stable fixed point of the renormalisation group [5]. We thus expect predictions made with the model (3), and in particular critical behaviour such as the value of  $N_{fc}$ , to be generally valid for Son's model (1) in the limit of large  $\lambda$ .

## 2. Lattice Simulations

The lattice model studied in this paper is related to the lattice Thirring model studied in [5], except that in this case we used the compact formulation for the auxiliary boson field. The simulations were performed with the standard hybrid molecular dynamics algorithm. The novelty of [7] is that it is the first study of the Thirring model by lattice simulations in the strong-coupling limit  $g^2 \rightarrow \infty$ . Since we aim to repeat the strategy here we should discuss how



**Figure 1.**  $\langle \bar{\psi}\psi \rangle$  vs.  $1/g^2$  near  $g_{\text{peak}}$  for  $N_f = 2$ .

this was done. First, note that the vacuum polarisation calculation leading to the results (2,4) does not go through in quite the same way for the lattice regularised model; rather, there is an additive correction which is momentum independent and UV-divergent:

$$\Pi^{\text{latt}}(p) = \Pi^{\text{cont}}(p) + g^2 J(m), \quad (5)$$

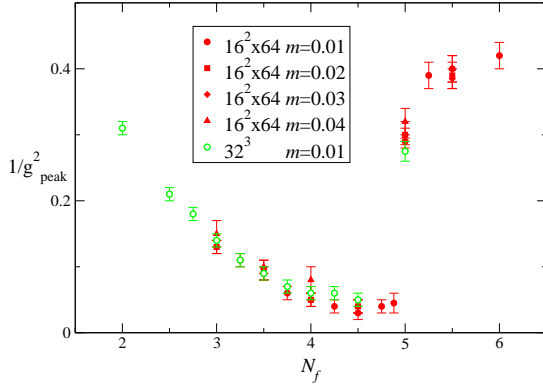
where  $J(m)$  comes from incomplete cancellation of a lattice tadpole diagram [5]. This extra divergence not present in the continuum treatments can be absorbed by a wavefunction renormalisation of  $V$  and a coupling constant renormalisation

$$g_R^2 = \frac{g^2}{1 - g^2 J(m)}. \quad (6)$$

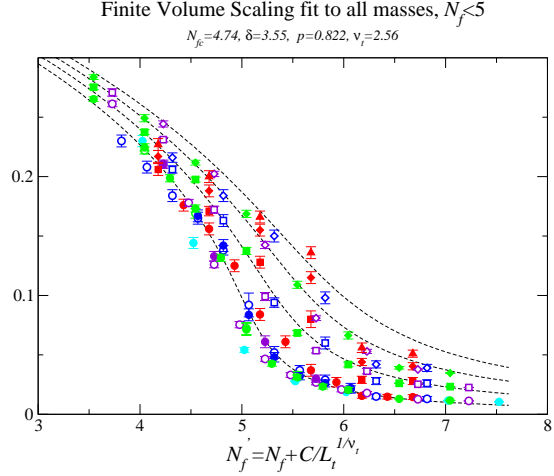
In the large- $N_f$  limit we thus expect to find the strong coupling limit of the lattice model at  $g_R^2 \rightarrow \infty$  implying  $g^2 \rightarrow g_{\text{lim}}^2$ . For  $g^2 > g_{\text{lim}}^2$   $D_{\text{latt}}(p)$  becomes negative, and  $S_{\text{latt}}$  no longer describes a unitary theory.

Away from the large- $N_f$  limit, where chiral symmetry may be spontaneously broken, there is no analytical criterion for identifying  $g_{\text{lim}}^2$ ; however in this case a numerical calculation of  $\langle \bar{\psi}\psi \rangle$  shows a clear peak at  $g^2 = g_{\text{peak}}^2$ , whose location is approximately independent of both volume and  $m$ , indicating an origin at the UV scale [7]. Fig. 1 exemplifies this behaviour in the lattice model with  $N_f = 2$  on system volumes  $L^3$ : for  $L \geq 24$  we identify  $1/g_{\text{peak}}^2 \simeq 0.3$ . Since for orthodox chiral symmetry breaking the magnitude of the condensate is expected to increase monotonically with the coupling strength, we interpret the peak as the point where unitarity violation sets in, ie.  $g_{\text{lim}}^2 \approx g_{\text{peak}}^2$ . We use simulations performed at  $g^2 = g_{\text{lim}}^2$  to explore the strong coupling limit, and find clear evidence for a chiral symmetry restoring phase transition at a well-defined  $N_{fc}$ . As shown in Fig. 2  $1/g_{\text{peak}}^2$  decreases as  $N_f$  increases from 2 to 4.75. Near  $N_f \approx 4.75$  the curve reaches a minimum, implying a significant change in the strong coupling behavior of the model. The rapid change in the value of the condensate at  $N_f \approx 4.9$  implies a significant change in the strong coupling behavior of the model. This can be a phase transition that separates a chirally broken from a chirally symmetric phase. Since our model has anisotropic interactions in the spatial and temporal directions the correlation lengths near the transition diverge with different exponents,  $\nu_s$  in the spatial directions, and  $\nu_t$  in the temporal direction. In this case a modified hyperscaling relation holds:

$$\nu_t + (d - 1)\nu_s = \gamma + 2\beta. \quad (7)$$



**Figure 2.**  $1/g_{\text{peak}}^2$  vs.  $N_f$ .



**Figure 3.** Equation of State fits to data generated with different fermion masses on different lattice sizes.

We carefully monitored the finite size effects in the spatial directions by comparing the values of the condensate at  $m = 0.01$ ,  $g_{\text{peak}}^2(N_f)$  extracted from simulations on  $16^2 \times 48$  and  $24^2 \times 48$  lattices. Our results show that finite  $L_s$  effects are negligible for  $L_s \geq 16$ . We fitted the data generated on several lattices with  $L_t = 16$ ,  $L_s = 48, 64$  and  $m = 0.01, \dots, 0.04$  to the following RG-inspired equation of state [5]:

$$m = A[(N_f - N_{fc}) + CL_t^{-\frac{1}{\nu_t}}]\langle\bar{\psi}\psi\rangle^p + B\langle\bar{\psi}\psi\rangle^\delta, \quad (8)$$

where  $p \equiv \delta - \beta^{-1}$ . The results show clearly that the model undergoes a second order quantum phase transition and the values of the most significant parameters are:  $N_{fc} = 4.74$ ,  $\delta = 3.55$ ,  $p = 0.822$ , and  $\nu_t = 2.56$ . The data and the fitted curves are shown in Fig. 3. The value of  $N_{fc} = 4.74$  is close to the value of  $N_f \approx 4.9$ , where a rapid change in the  $1/g_{\text{peak}}^2$  vs  $N_f$  occurs.

### 3. Summary

We presented results from a non-perturbative Monte Carlo study of a Thirring-like model pertinent to graphene. Our analysis of its equation of state at strong coupling reveals that the model undergoes a second order quantum phase transition at  $N_{fc} \approx 4.74$ , which is greater than the physical  $N_f = 2$  value. This result implies that freely suspended graphene may be an insulator for couplings  $g$  larger than a critical coupling  $g_c$ .

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